

Optimized Perturbation Theory for Wave Functions of Quantum Systems

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Abstract

The notion of the optimized perturbation, which has been successfully applied to energy eigenvalues, is generalized to treat wave functions of quantum systems. The key ingredient is to construct an envelope of a set of perturbative wave functions. This leads to a condition similar to that obtained from the principle of minimal sensitivity. Applications of the method to quantum anharmonic oscillator and the double well potential show that uniformly valid wave functions with correct asymptotic behavior are obtained in the first-order optimized perturbation even for strong couplings.

PACS numbers: 03.65.Ge, 02.30.Mv, 11.15.Bt, 11.15.Tk

Naive perturbative expansions are usually divergent asymptotic series [1]. Thus various summation techniques such as the Borel and Padé methods have been developed [2]. In recent years, a new summation method “optimized perturbation theory (OPT)” has been studied. This combines straightforward perturbation with a variational principle and improves even the Borel non-summable series. Variants of OPT are called in various names, the (optimized) δ -expansion, the variational perturbation, the renormalized strong coupling expansion, and so on [3]. One of the key ingredients in the method is the principle of minimal sensitivity (PMS) [4], which says that physical quantities calculated in perturbation theory should not depend on any parameters absent in the original Hamiltonian.

The method has been applied to improve the energy eigenvalues of the quantum anharmonic oscillator (AHO) and the double-well potential (DWP); AHO and DWP are the useful laboratories to test a new non-perturbative method. A rigorous proof has been also given for the convergence properties of the perturbation series for energy eigenvalues of AHO/DWP [5]. The method is also being extensively applied to perturbation series for energy and partition functions in quantum field theories [6].

To the best of our knowledge, the wave functions has never been explored in OPT even for simple quantum mechanical problems. Needless to say, wave functions have all information of the system in question, including the energy eigenvalues. The purpose of this Letter is to show a novel generalization of the idea of the optimized perturbation for studying the wave functions.

Let's take the following Schrödinger equation for one dimensional AHO/DWP;

$$\frac{1}{2}\left(-\frac{d^2}{dx^2} \pm x^2 + \lambda x^4\right)\psi_n(x) = E_n(\lambda)\psi_n(x). \quad (1)$$

Naive Rayleigh-Schrödinger (RS) expansion for eigenvalues $E(\lambda) = \sum_n \lambda^n C_n$ gives an asymptotic series with coefficients growing as $C_n \sim n!$ [7]. A scaled Hamiltonian in the simplest version of OPT (sometimes called the linear δ -expansion) reads $H_\delta = H_0(\Omega) + \delta \cdot H_I(\Omega, \lambda)$ with

$$H_0(\Omega) = \frac{1}{2}\left(-\frac{d^2}{dx^2} + \Omega^2 x^2\right), \quad (2)$$

$$H_I(\Omega, \lambda) = \frac{1}{2} \left((\pm 1 - \Omega^2)x^2 + \lambda x^4 \right). \quad (3)$$

H_δ interpolate the free Hamiltonian with a frequency Ω and the full Hamiltonian; $H_{\delta=0} = H_0(\Omega)$ and $H_{\delta=1} = H$. The essential idea of OPT is to choose a suitable Ω so that the RS perturbation $E(\lambda) = \sum_n \delta^n C_n$ becomes a convergent series with errors exponentially suppressed for large n . PMS in this case is one of the possible criteria for choosing Ω , although it is not a unique one [4].

To show how the naive application of the idea of OPT to the wave function fails, we first expand the wave function of H_δ by the eigenfunctions of H_0 ,

$$\psi_k(x; \Omega) = \sum_j C_{jk}(\Omega) \psi_j^0(x; \Omega). \quad (4)$$

$C_{jk}(\Omega)$ is evaluated in the RS perturbation theory with δ being an expansion parameter, $C_{jk}(\Omega) = C_{jk}^0 + \delta \cdot C_{jk}^1 + \dots$. With a suitable Ω , one might expect $\psi(x, \Omega)$ at $\delta = 1$ converges rapidly to the exact wave function $\psi^{\text{exact}}(x)$ as in the case of the energy eigenvalues E . However, this is not the case as long as Ω is independent of x . In fact, in any finite orders of the expansion in (4), $\psi_n(x \rightarrow \infty; \Omega) \sim \exp(-\Omega x^2/2)$, while the exact wave function in (1) behaves as

$$\psi^{\text{exact}}(x \rightarrow \infty) \sim \exp\left(-\sqrt{\frac{\lambda}{9}} |x|^3\right). \quad (5)$$

Thus, the series (4) can never reproduce the true asymptotic behavior no matter what Ω is chosen as long as Ω is constant.

To find a way out, let us describe the situation in geometrical terms. The perturbative wave function (4) with constant Ω gives a locally valid approximation around certain x where the perturbation $\delta \cdot H_I(\Omega)$ is sufficiently small; however, this is not a uniformly valid solution in the entire domain of x . Conversely speaking, if Ω is varied, we have a family of functions $\{\psi(x; \Omega)\}_\Omega$ parametrized with Ω , each of which is locally valid around certain x . Therefore a uniformly valid wave function may be constructed as an envelope of the family of perturbative ones. To obtain an equation to determine the envelope, we recall the

classical theory of envelopes [8]: Suppose one has a set of functions $f(x; \alpha)$ parametrized by α . Then the envelope of $\{f(x; \alpha)\}_\alpha$ can be obtained by solving $\partial f(x; \alpha)/\partial \alpha = 0$ and substituting the solution $\alpha(x)$ into the original function i.e. $f(x; \alpha(x))$. In our case, $f = \psi$ and $\alpha = \Omega$. Thus we reach a condition,

$$\left. \frac{\partial \psi(x; \Omega)}{\partial \Omega} \right|_{\delta=1} = 0. \quad (6)$$

This condition has another interpretation in term of PMS: The exact wave functions of (1) do not depend on the fictitious PMS parameter Ω at $\delta = 1$. So one would impose the condition that even the approximate wave function should not depend on Ω , which leads to eq.(6). A similarity of this idea to that of the renormalization group à la Gell-Mann-Low is also to be noted.

At this point, one may ask whether $\psi(x; \Omega(x))$ thus obtained satisfies the original Schrödinger equation where d/dx acts on $\Omega(x)$ too: $(d/dx)\psi(x; \Omega(x)) = (\partial/\partial x)\psi(x; \Omega(x)) + (\partial\Omega(x)/\partial x) \cdot (\partial/\partial \Omega)\psi(x; \Omega(x))$. The answer is yes, since the second term vanishes on account of the condition (6). The same is true for d^2/dx^2 . Hence the improved wave function satisfies the Schrödinger equation at every point x at least up to the same order of the δ -expansion employed.

Solution of (6) gives Ω as a function of x (and λ). For AHO/DWP, eq. (6) turns out to be an algebraic one. The envelope wave function $\psi(x; \Omega(x))$ obtained by substituting the solution of (6) into (4) turns out to be a uniformly valid approximation for $\psi^{\text{exact}}(x)$ in a global domain even in the lowest order of the δ -expansion.

Let us demonstrate the above points explicitly for AHO/DWP with the first order δ -expansion in which $C_{jk} = \delta_{jk} - \langle j | H_I | k \rangle / (E_j^0 - E_k^0)$. The condition eq. (6) gives an algebraic equation for Ω as

$$\begin{aligned} \Omega(\pm 1 - \Omega^2) \left(A_n H_n(\sqrt{\Omega}x) + 4n(n-1)A_{n-2}H_{n-2}(\sqrt{\Omega}x) \right) \\ + \lambda \cdot \left(B_n H_n(\sqrt{\Omega}x) + 4n(n-1)B_{n-2}H_{n-2}(\sqrt{\Omega}x) \right) = 0, \end{aligned} \quad (7)$$

where $H_n(z)$ is the n -th Hermite polynomial, and the functions $A_n(\sqrt{\Omega}x)$ and $B_n(\sqrt{\Omega}x)$

are given as follows; $A_n(z) = 16z^4 - 16(2n - 1)z^2 - 4(8n + 7)$, $A_{n-2}(z) = -16$, $B_n(z) = 8z^6 + 4(2n + 9)z^4 - 2(24n^2 + 4n - 33)z^2 - 9(8n^2 + 26n + 11)$, and $B_{n-2}(z) = -2(8z^2 + 18n + 9)$.

Several remarks on Eq.(7) are in order here.

1. Eq.(7) gives an algebraic equation of degree $m + 5$ for Ω with $n = 2m$ or $2m + 1$. As in the usual PMS condition applied to the energy eigenvalues, one needs some principle to select a relevant root. The true solution $\Omega(x)$ is selected so that the local energy $\mathcal{E}_n(x)$ defined by $\psi(x; \Omega(x))^{-1} H \psi(x; \Omega(x))$ is (roughly) constant as a function of x .
2. For $\lambda = 0$, there is an obvious solution $\Omega(x) = 1$ for (7). Other solutions do not satisfies $\mathcal{E}_n(x) \simeq \text{constant}$.
3. For $x \rightarrow \infty$, eq.(7) with an ansatz $\Omega(x) \sim Cx^p$ ($p > 0$) gives an equation independent of n . It has a solution $C^2 = \lambda/2$ and $p = 1$. Thus the asymptotic form reads

$$\psi(x; \Omega(x)) \rightarrow \exp(-\sqrt{\frac{\lambda}{8}} |x|^3) \quad (8)$$

which has a same asymptotic behavior with (5). This feature is never obtained by any finite-order RS perturbation as we mentioned. A slightly different numerical coefficient of $|x|^3$ is to be improved with higher order δ -expansion [9].

4. Although $\psi(x; \Omega)$ with constant Ω is normalized as $\int_{-\infty}^{\infty} |\psi(x; \Omega)|^2 dx = 1$, the norm of $\psi(x; \Omega(x))$ deviates from unity due to the x dependence of Ω . In the following figures, we will always show renormalized wave functions.

In fig. 1, the real and positive solutions of (7) for the ground state of AHO with intermediate coupling ($\lambda = 1$) are shown as a function of x . The local energy is approximately constant for the branch I. In the interval $0.684 \leq x \leq 0.780$, $\Omega(x)$ becomes complex with a small imaginary part. When we construct a continuous wave function in this interval, we adopt a real part of $\Omega(x)$ as a simplest way of interpolation [11]. We expect that the width of this interval and the associated small imaginary part of $\Omega(x)$ will vanish in the higher order δ -expansion. This must be, however, checked explicitly, which is now under progress.

In fig. 2, the ratio $R \equiv \psi(x; \Omega(x))/\psi^{\text{exact}}(x)$ as well as $\psi(x; \Omega(x))$ for the ground state of AHO are shown for intermediate coupling ($\lambda = 1$) and strong coupling ($\lambda = 100$). $\psi^{\text{exact}}(x)$

is numerically solved in double precision using the shooting method with FORTRAN [12].

It is not until x exceeds $x_c = 2.725(1.211)$ for $\lambda = 1(100)$ that the relative error of $\psi(x; \Omega(x))$ to the exact one becomes more than 10%. Such a value of x_c is large enough in the sense that the absolute value of the wave function at x_c is already as tiny as $\psi(x_c) = 0.00016(0.0012)$. Hence our first order results can be used as an exact one for practical use of the wave function. In fig. 2, $O(1)$ deviation is seen for quite large values of x . This is due to the approximate asymptotic behavior of $\psi(x; \Omega(x))$. The ratio R for large x can be estimated from (5) and (8) as $R \sim \exp(-0.02\sqrt{\lambda} |x|^3)$.

To see the accuracy of the wave function more quantitatively, a comparison of $\psi^{\text{exact}}(x)$ and $\psi(x; \Omega(x))$ for $\lambda = 100$ is shown in Table I for the ground state of AHO.

As we have mentioned before, $\psi(x; \Omega(x))$ is the envelop of the perturbative wave functions parametrized by Ω . In fig. 3, thin lines are the wave functions for $\lambda = 1$ with constant Ω varied. There are two envelopes of this family of wave functions, which are labeled by I and II in the figure. $\psi(x; \Omega(x))$ is obtained by the envelop I.

In Table II, expectation values of several operators including the full Hamiltonian H with respect to $\psi(x; \Omega(x))$ are compared with the exact numbers. The agreement is excellent as a first-order approximation.

Some final remarks are in order here.

1. Although we have shown only the ground state wave function because of the limitation of space, we have also studied the excited states ($n \neq 0$) and found that $\psi(x; \Omega(x))$ are as good approximation for $\psi^{\text{exact}}(x)$ as the $n = 0$ case.
2. The present method here can be used to study the double well potential where the sign of the x^2 term in (1) is negative. In the first order δ -expansion, we have found that the exact wave function is accurately reproduced for strong couplings, but the approximation breaks down qualitatively for $\lambda < 0.065$. In such weak couplings, or equivalently a high barrier at the origin, the ground state wave function is well localized in the two degenerate minima of the double well potential. Therefore, it is natural to expect that the naive δ -expansion scheme using $H_0(\Omega)$ with a single harmonic potential does not work. An introduction of a

new PMS parameter is under investigation to widen the applicability of the method.

3. We have also performed the second order δ -expansion for AHO. The formula is more lengthy and the degree of the algebraic equation is higher. The detailed comparison with the first order result is under progress.

4. Applications to other quantum mechanical system such as the scattering problem, Zeeman effect, and Stark effect [1] are interesting. Also, applications to field theory such as the improvement of the space-time (or momentum) dependence of Green's functions are closely related to the problem studied in this work.

5. The notion of envelopes has been found useful for global asymptotic analysis of some of ordinary/partial differential equations having *secular terms* in perturbative solutions [10]. The present work together with those in [10] shows that the notion of envelopes can be a useful guide for the improvement of perturbative expansions and asymptotic analyses. [13]

In summary, we have developed an optimized perturbation theory for wave functions for AHO and DWP. The optimized wave functions are constructed as an envelope of perturbative ones, and the principle of minimal sensitivity can be regarded as a condition for constructing envelopes. The optimized wave function thus obtained in the first-order δ -expansion has a correct asymptotic behavior at $x \rightarrow \infty$ and is uniformly valid for entire domain of x even for the strong coupling.

ACKNOWLEDGEMENTS

The authors thank H. Kitagawa for his help of solving the Schrödinger equation numerically in high accuracy. This work was supported by the Grants-in-Aid of the Japanese Ministry of Education, Science and Culture (No. 06102004), (No. 07304065) and (No. 08640396).

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They obtain the asymptotic form of the wave function (5) only after further resummation. Relation between our approach and theirs is not clear.

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- [13] The improved energy eigenvalue obtained by PMS in previous works may be interpreted as an envelope $E(\lambda; \Omega(\lambda))$ of a set of perturbative energy eigenvalues $\{E(\lambda; \Omega)\}_\Omega$.

FIGURES

FIG. 1. $\Omega(x)$ as roots of the algebraic equation for the ground state with intermediate coupling $\lambda = 1$. The branch I gives approximately constant local-energy.

FIG. 2. The ratio $R \equiv \psi(x; \Omega(x))/\psi^{\text{exact}}(x)$ as well as $\psi(x; \Omega(x))$ itself for the ground state. The solid (dashed) line is for the intermediate (strong) coupling $\lambda = 1(100)$.

FIG. 3. Family of perturbative wave functions with constant Ω with $0.1 \leq \Omega \leq 100$ for the ground state with $\lambda = 1$. Thick lines labeled as I and II are their envelopes.

TABLES

	$x = 0.0$	$x = 0.5$	$x = 1.0$	$x = 1.5$	$x = 2.0$
$\psi(x; \Omega(x))$	1.170E0	5.519E-1	1.885E-2	3.925E-6	3.095E-13
$\psi^{\text{exact}}(x)$	1.167E0	5.564E-1	1.979E-2	5.168E-6	7.982E-13

TABLE I. Ground state wave functions of AHO for $\lambda = 100$; $\psi(x; \Omega(x))$ is an approximate wave function in the first order δ -expansion.

		$\langle p^2 \rangle$	$\langle x^2 \rangle$	$\langle x^4 \rangle$	$\langle H \rangle$
$\lambda = 1$	PMS	0.83146	0.30391	0.25703	0.69620
	Exact	0.82630	0.30581	0.26024	0.69618
$\lambda = 100$	PMS	3.34430	0.07641	0.01579	2.50003
	Exact	3.30717	0.07731	0.01615	2.49971

TABLE II. Expectation values of $p^2 = (-id/dx)^2$, x^2 , x^4 and the full Hamiltonian H for the ground state in AHO.

Fig.1

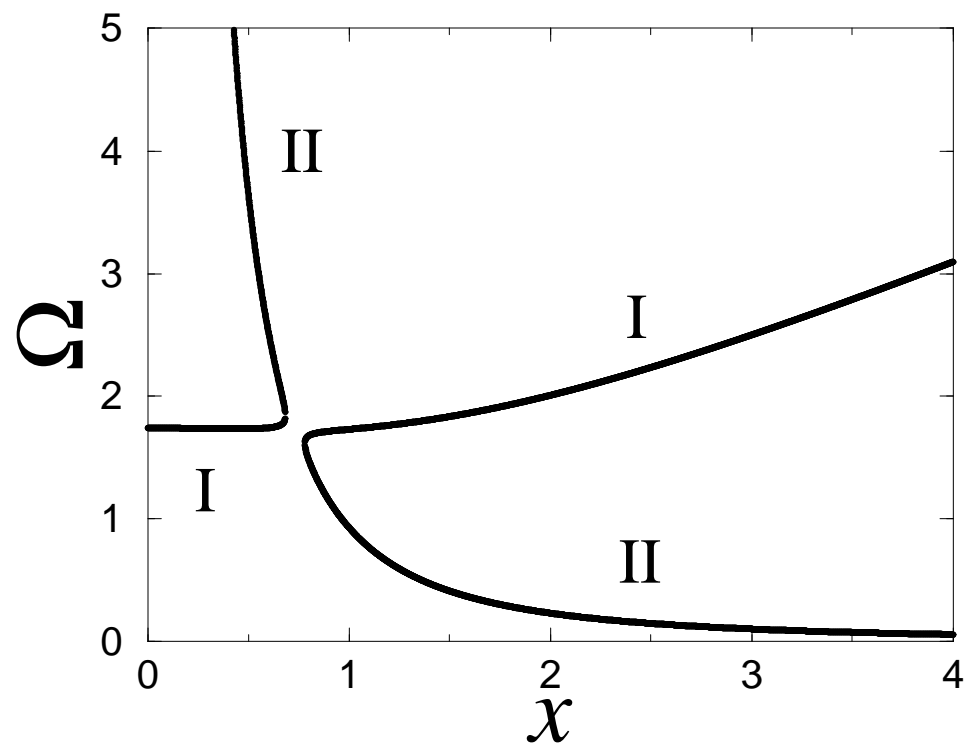


Fig.2

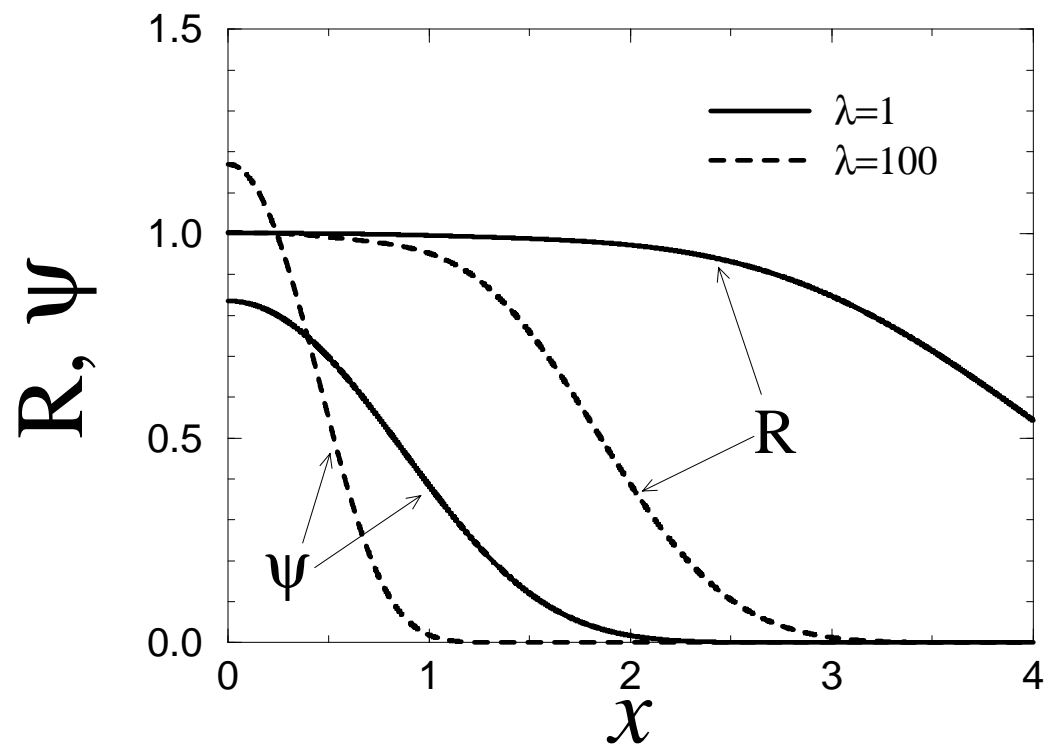


Fig.3

